

Petrus H. Zwart

CONTACT INFORMATION	1 Cyclotron Road Bldg 64, Room 246B Berkeley Nat. Laboratories Berkeley, 94720 CA, USA	<i>home phone:</i> +1 510 717 0169 <i>work fax:</i> +1 510 486 6341 <i>work phone:</i> +1 510 486 5909 <i>email:</i> PHZwart@lbl.gov
STATUS	Date and place of birth Sex Marital Status Nationality	May 10, 1976, Anna Paulowna, The Netherlands Male Married Dutch
RESEARCH INTERESTS	General Crystallographic Methods, (Bayesian) Statistics, Protein and Small Molecule Crystallography, Powder Diffraction, Structural Biology.	
EDUCATION AND RESEARCH	September 1994 – August 1999 November 1997 – Februari 1998 December 1998 – March 1999 September 1999 – August 2003 September 2003 – October 2003 Februari 2004 – November 2005 November 2004 – March 2005 March 2005 – Present	M.Sc. Chemistry, University of Amsterdam, Faculty of Chemistry, Laboratory of Crystallography. Research project at the European Molecular Biology Laboratory (EMBL) in the group of Dr. V.S. Lamzin on the structure solution and refinement of SS-LADH. Research project at the European Synchrotron Radiation Facility (ESRF) in the group of Dr. H. Graafsma on the crystal structure of deuterated Potassium Phosphate in a static electric field. PhD-student at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin. Home institute and supervisor: University of Amsterdam, Prof. Dr. H. Schenk. Defense date: December 17, 2003. Postdoctoral fellow at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin. Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the NSLS, Brookhaven National Laboratories, Upton NY, USA Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the Argonne National Laboratories, Argonne, IL, USA Postdoctoral fellow in the group of Dr. Adams, Lawrence Berkeley National Laboratories, Berkeley, CA.
AWARDS AND FELLOWSHIPS	June 1999 October 2000	EMBL Fellowship to carry out PhD-research in the group of Dr. Lamzin. Unilever Research Price for undergraduate work.

PUBLICATIONS

- Zwart, P.H.** (2005). Anomalous signal indicators in protein crystallography, *Acta Cryst. D* **61** In the press.
- Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adams, P.D. (2005). Characterisation of X-ray data sets, *CCP4 newsletter* **42**, contribution 10.
- Zwart, P.H.**, Langer G.G. & Lamzin, V.S. (2004). Modelling Bound ligands in protein crystal structures, *Acta Cryst. D* **60**, 2230–39
- Zwart, P.H.**, Banumathi, S., Dauter, M. & Dauter, Z. (2004). Radiation-damage-induced phasing with anomalous scattering: substructure solution and phasing, *Acta Cryst. D* **60**, 1958–63.
- Banumathi, S., **Zwart, P.H.**, Ramagopal, U.A., Dauter, M. & Dauter Z. (2004). Structural effects of radiation damage and its potential for phasing, *Acta Cryst. D* **60**, 1085–93.
- Zwart, P.H.** & Lamzin, V.S. (2004). The influence of positional errors on the Debye effects, *Acta Cryst. D* **60**, 220–6.
- Zwart, P.H.** (2003). Error Estimation and Pattern Recognition Techniques in Protein Crystallography. (PhD Thesis).
- Zwart, P.H.** & Lamzin, V.S. (2003). Distance distributions and electron density characteristics of protein models, *Acta Cryst. D* **59**, 2104–13..
- Morris, R.J., **Zwart, P.H.**, Cohen, S., Fernandez, F.J., Kakaris M., Kirillova, O., Vonrhein, C., Perrakis, A. & Lamzin, V.S. (2003). Breaking good resolutions with ARP/wARP, *J. Synch. Rad.* **11**, 56–9.
- Lorentzen, E., Pohl, E., **Zwart, P.**, Stark, A., Russell, R.B., Knura, T., Hensel, R., Siebers, B. (2003). Crystal structure of an archaeal class I aldolase and the evolution of $(\beta\alpha)8$ barrel proteins. *J Biol Chem.* **278**, 47253–60
- Pegasova, T.V., **Zwart P.H.**, Koroleva O.V., Stepanova E.V., Rebrikov D.V. & Lamzin V.S. (2003). Crystallization and preliminary X-ray analysis of a four-copper laccase from *Coriolus hirsutus*. *Acta Cryst. D* **59**, 1459–61.
- Van Langevelde, A., Van Malssen, K., Driessen, R., Goubitz, K., Hollander, F., Peschar R., **Zwart P.**, & Schenk H. (2000). Structure of CnCn+2Cn-type (n = even) beta'-triacylglycerols. *Acta Cryst. B* **56** 1103–11.
- Adolph H.W., **Zwart, P.**, Meijers, R., Hubatsch, I., Kiefer, M., Lamzin, V., Cedergren-Zeppezauer, E. (2000). Structural basis for substrate specificity differences of horse liver alcohol dehydrogenase isozymes. *Biochemistry* **39** 12885–97.

NON
PEER-REVIEWED
ARTICLES

- Banumathi, S., **Zwart, P.H.**, Dauter, M., Dauter, Z., (2004) Structural effects of radiation damage and its potential for phasing, *National Synchrotron Light Source Science Highlights*, November 5, 2004. (<http://www.nsls.bnl.gov/newsroom/science/2004/11-Dauter.htm>).
- Zwart, P.H., Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Characterization of X-ray data sets. *CCP4 Newsletter No. 42*.
- Zwart, P.H., Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Xtriage and Fest: automatic assessment of X-ray data and substructure structure factor estimation. *CCP4 newsletter No. 43*

Zwart, P.H., Grosse-Kunstleve, R.W. & Adam, P.D. (2006) Exploring Metric Symmetry. CCP4 newsletter No. 44

ORAL
PRESENTATIONS

Coordinate Error estimation of a set of free atoms, XIXth International Union of Crystallography Conference and General Assembly, August 6–15, 2002, Geneva, Switzerland (Invited Speaker).

Automated Ligand building in ARP/wARP, Current Trends in Structure Aided Drug Design, May 22–24, 2003, Lund, Sweden (Invited Speaker).

Ligand Fitting, CCP4 Study Weekend 2004, Januari 4–5, 2004, Leeds, United Kingdom (Invited Speaker).

Tutor in CCP4 workshop on computational crystallographic methods in Bangalore, India, March 15–20, 2005.

Radiation damage induced phasing with anomalous scattering, ACA annual meeting, May 28 – June 2, 2005, Orlando, USA (Invited speaker).

First aid and Pathology; Data quality assessment with Xtriage International Symposium on Recent Trends in Macromolecular Structure and Function, January 18–20, 2006, Chennai, Tamil Nadu, India (Invited speaker).

Data quality assessment with Xtriage, Gordon research conference on Diffraction Methods in Structural Biology, June 16–21, Lewiston, USA.

POSTER
PRESENTATIONS

Modelling Bound ligands in protein crystal structures. Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA

Radiation-damage induced phasing with anomalous scattering. Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA

SKILLS

Languages

Dutch: Mother tongue, English: Fluent, German: Good

Operating systems

working knowledge of UNIX, LINUX, Windows and Mac OSX

Programming

Working knowledge of C++ and python, Limited knowledge of Fortran.

Approximately 1.5 years experience with the open source CCTBX crystallographic libraries (<http://cctbx.sf.net>).

Crystallographic Software

Experience with most Crystallographic software,
notably HKL2000/Denzo/Scalepack, Best, Solve/Resolve, SHARP, SHELXD, SnB, CCP4.

Synchrotron Crystallography

Performed experiments on most crystallographic beamlines at the EMBL-Hamburg outstation.
Conducted user support and experiments on NSLS beamline X9B.

Other

Working knowledge of L^AT_EX.